

Interaction Potential for Inert Gas Mixtures

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Possible applications of the three-parameter internuclear potential functions (Morse, Frost-Musulin and the others) have been demonstrated in a number of papers (i). Derivation of the Frost-Musulin pair potential, within the pseudopotential scheme, is valid when interacting particles are identical (ii). Such a scheme permits one to obtain generalized expressions valid for the pair interaction of different pseudoatoms too. In this case, potential functions contain six parameters: effective ion charges, effective screening constants and ion core radii. Observed quantities: dissociation energy from the bottom of the potential curve, bond-length and vibration frequency are explicit functions of the pseudopotential parameters mentioned. Numerical estimation shows that each observed quantity and internuclear distance at which the "mixed" potential vanishes, may be equated to the average between analogous quantities characterizing interaction of identical atoms. Second and higher derivatives of the generalized potential function are examined too.

(i) D.Steele, E.Lippincott and J.Vanderslice, Rev. Mod. Phys. V. 34, 239 (1962).

(ii) N.V.Fomin, International Workshop on New Approaches to High - Tech. Materials: Nondestructive Testing and Computer Simulation in Material Science and Engineering. A.I.Melker, Editor, Proceeding of SPIE Vol. 3345, 106 (1998).